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# Generalization of Gutzwiller Approximation

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(Received January 20, 1997 )

We derive expressions required in generalizing the Gutzwiller approximation to models comprising arbitrarily degenerate localized orbitals.

KEYWORDS: Gutzwiller approximation, degenerate-band model

Previously, we generalized the Gutzwiller approximation to degenerate-band models, and investigated itinerant ferromagnetism in the $3d$ transition metal systems.[1)] There, we presented the resulting formula but omitted its derivation because it was quite complicated.[2)] However, once we know the physical interpretation of the result as explained in ref. 1, it is natural to expect that the formula may be derived rather straightforwardly in the way that it reflects the simple interpretation. In fact, as we found this is actually the case, we report it in the following. At the end, we show that the Brinkman-Rice transition occurs only when the carrier density equals an integer.

We investigate the Hamiltonian comprising arbitrary numbers of localized orbitals $l$;

$$H = T + V = \sum_{i,j,l} t^l_{ji} c^\dagger_{jl} c_{il} + \sum_i \sum_{\substack{p \\ \{l_1,\cdots,l_p\}}} C^{(p)}(l_1,\cdots,l_p)\hat{\nu}^{(p)}_i(l_1,\cdots,l_p). \tag{1}$$

For simplicity, the hopping part $T$ is assumed to be diagonal with respect to $l$. In the potential part $V$, indices $l_m$ designate orbital and spin of localized states. Operators $\hat{\nu}^{(p)}_i(l_1,\cdots,l_p)$ have eigenvalue 1 if only $p$ orbitals $l_1,\cdots,l_p$ are occupied (the others unoccupied) at site $i$. These operators correspond to $\hat{d}_i \equiv \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$ of the single band Hubbard model. The sum in $V$ is taken over a set $\{l_1,\cdots,l_p\}$, not to count their combination redundantly. The Pauli principle requires $l_m \neq l_n$ for $m \neq n$ for the orbitals in the braces $\{l_1,\cdots,l_p\}$. $C^{(p)}(l_1,\cdots,l_p)$ is interaction energy of an eigenstate of $\hat{\nu}^{(p)}_i(l_1,\cdots,l_p)$. Generalizing the Gutzwiller approx-

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imation, we can estimate the expectation value of $H$ as

$$\frac{1}{L}\langle\Psi|H|\Psi\rangle = \sum_l q(l)\tilde{\varepsilon}_l + \sum_{\substack{p \\ \{l_1,\cdots,l_p\}}} C^{(p)}(l_1,\cdots,l_p)\nu^{(p)}(l_1,\cdots,l_p), \tag{2}$$

where $\tilde{\varepsilon}_l$ is defined by

$$\tilde{\varepsilon}_l \equiv \frac{1}{L}\langle\Psi_0|\sum_{i,j} t_{ji}^l c_{jl}^\dagger c_{il}|\Psi_0\rangle, \tag{3}$$

and represents the average kinetic energy of the band $l$ for the uncorrelated state $|\Psi_0\rangle$, for which we assume $\langle\Psi_0|\Psi_0\rangle = 1$. In eqs. (2) and (3), $L$ is the total number of lattice sites. Parameters $\nu^{(p)}(l_1,\cdots,l_p)$ are the expectation value of $\hat{\nu}_i^{(p)}(l_1,\cdots,l_p)$, and take non-negative values. In the uncorrelated case, where $C^{(p)} = 0$ for any $p$, these are given by

$$\nu^{(p)}(l_1,\cdots,l_p) = \nu_0^{(p)}(l_1,\cdots,l_p) \equiv \prod_{i=\{1,\cdots,p\}} n(l_i) \prod_{i\neq\{1,\cdots,p\}} (1-n(l_i))\,, \tag{4}$$

where

$$n(l) \equiv \frac{1}{L}\langle\Psi_0|\sum_i c_{il}^\dagger c_{il}|\Psi_0\rangle. \tag{5}$$

Most difficult and laborious part in applying the Gutzwiller approximation is the calculation of the band-width reduction factor $q(l)$ in eq. (2) as a function of $\nu^{(p)}(l_1,\cdots,l_p)$. If this is achieved, $\nu^{(p)}(l_1,\cdots,l_p)$ are determined so as to minimize $\langle\Psi|H|\Psi\rangle$. In the variational calculation, these parameters $\nu^{(p)}$ cannot take arbitrary values since they must satisfy two relations,[1] i.e., 'conservation of number',

$$n(l_1) = \nu^{(1)}(l_1) + \sum_{p(\geq 2)} \sum_{\{l_2,\cdots,l_p\}(\neq l_1)} \nu^{(p)}(l_1,l_2,\cdots,l_p), \tag{6}$$

and 'conservation of probability',

$$\sum_p \sum_{\{l_1,\cdots,l_p\}} \nu^{(p)}(l_1,\cdots,l_p) = 1. \tag{7}$$

Therefore for fixed $n(l_i)$ we must regard only $\nu^{(p)}$ with $p \geq 2$ as variational parameters.

A general result for $q(l)$ was obtained for the first time in ref. 1,

$$q(l_1) = \frac{1}{n(l_1)\,(1-n(l_1))} \left( \sum_{p\geq 1} \sum_{\{l_2,\cdots,l_p\}(\neq l_1)} \sqrt{\nu^{(p)}(l_1,\cdots,l_p)}\sqrt{\nu^{(p-1)}(l_2,\cdots,l_p)} \right)^2, \tag{8}$$

and interpreted physically as shown in Fig. 1. Terms in the round bracket squared are interpreted as a sum ($\sum_p$) of products ($\sqrt{\nu^{(p)}}\sqrt{\nu^{(p-1)}}$) of probability amplitudes ($\sqrt{\nu^{(p)}}$), which are involved in the hopping process under consideration. The square is due to contributions from two sites $i$ and $j$. One can make sure that $\nu_0^{(p)}(l_1,\cdots,l_p)$ defined in eq. (4) meet eqs. (6) and (7), and thus verify that $q(l) = 1$ for $C^{(p)} = 0$ using eq. (7), as expected. To

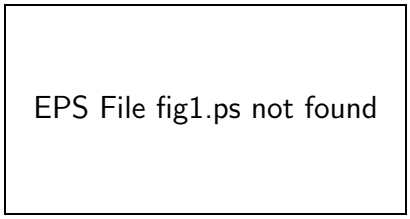


Fig. 1. Examples of the hopping process. A carrier in the orbital $l_1$ at site $i$ moves to the orbital $l_{1'}$ at site $j$.

derive eq. (8), we must derive relations between $\nu^{(p)}$ and the Gutzwiller projection factors $\eta^{(p)}$ ($\leq 1$), which are defined in the generalized Gutzwiller wavefunction,

$$|\Psi\rangle = \prod_{\substack{i \\ p,\{l_1,\cdots,l_p\}}} \left[1 - \left(1 - \eta^{(p)}(l_1,\cdots,l_p)\right) \hat{\nu_i}^{(p)}(l_1,\cdots,l_p)\right] |\Psi_0\rangle, \tag{9}$$

where $\eta^{(1)}(l_i) \equiv \eta^{(0)} \equiv 1$.

In the Gutzwiller approximation, the norm of the state (9) is estimated as

$$\langle\Psi|\Psi\rangle = \prod_{\substack{p \\ \{l_1,\cdots,l_p\}}} \sum_{\bar{\nu}^{(p)}} \left[\eta^{(p)}(l_1,\cdots,l_p)\right]^{2\bar{\nu}^{(p)}(l_1,\cdots,l_p)} N\left(L, \{N(l_i)\}, \{\bar{\nu}^{(p)}\}\right) P\left(L, \{N(l_i)\}\right), \tag{10}$$

where

$$\begin{aligned} \bar{\nu}^{(p)}(l_1,\cdots,l_p) &\equiv L\,\nu^{(p)}(l_1,\cdots,l_p), \\ N(l_i) &\equiv L\,n(l_i), \\ N\left(L, \{N(l_i)\}, \{\bar{\nu}^{(p)}\}\right) &= \frac{L!}{\displaystyle\prod_{\substack{p \\ \{l_1,\cdots,l_p\}}} \bar{\nu}^{(p)}(l_1,\cdots,l_p)\,!}, \\ P\left(L, \{N(l_i)\}\right) &= \prod_i n(l_i)^{N(l_i)} \left(1 - n(l_i)\right)^{L - N(l_i)}. \end{aligned} \tag{11}$$

These are generalization of the results of Vollhardt[3] for the single band model.

Then, we shall approximate the sum over $\bar{\nu}^{(p)}$ in eq. (10) by a single term which gives the largest contribution in the thermodynamic limit $L \to \infty$; $\bar{\nu}^{(p)}$ ($p \geq 2$) is determined by

$$\frac{\mathrm{d}}{\mathrm{d}\bar{\nu}^{(p)}(l_1,\cdots,l_p)} \log\langle\Psi|\Psi\rangle = 0, \tag{12}$$

from which we obtain a relation between $\eta^{(p)}(l_1,\cdots,l_p)$ and $\nu^{(p)}(l_1,\cdots,l_p)$,

$$\left[\eta^{(p)}(l_1,\cdots,l_p)\right]^2 = \frac{(\nu^{(0)})^{p-1}\nu^{(p)}(l_1,\cdots,l_p)}{\nu^{(1)}(l_1)\cdots\nu^{(1)}(l_p)}. \tag{13}$$

To derive eq. (13) from eqs. (10) and (12), one may note

$$\frac{\mathrm{d}\bar{\nu}^{(1)}(l_i)}{\mathrm{d}\bar{\nu}^{(p)}(l_1,\cdots,l_p)} = -1, \qquad (i=1,\cdots,p)$$
$$\frac{\mathrm{d}\bar{\nu}^{(0)}}{\mathrm{d}\bar{\nu}^{(p)}(l_1,\cdots,l_p)} = p-1, \tag{14}$$

owing to eqs. (6) and (7), and

$$\frac{\mathrm{d}}{\mathrm{d}N}\log N! = \log N. \qquad (N\to\infty) \tag{15}$$

As a next step, we note that spatial correlation of various configurations is completely neglected in the Gutzwiller approximation. Thus, the factor $q$ can be separated into two independent parts, each of which comes from contribution for the creation and annihilation operators;

$$\frac{\langle\Psi|c^{\dagger}_{jl_{1'}}c_{il_1}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \to r_{c^{\dagger}_{l_{1'}}}\, r_{c_{l_1}} \frac{\langle\Psi_0|c^{\dagger}_{jl_{1'}}c_{il_1}|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}. \tag{16}$$

To calculate $r_{c_{l_1}}$ for the process shown in Fig. 1, two factors appear besides the Gutzwiller parameters $\eta^{(p)}\left(\{l_1,\cdots,l_p\}\right)\eta^{(p-1)}\left(\{l_2,\cdots,l_p\}\right)$. These are the following ratios, i.e.

$$\frac{N\left(L-1,N(l_1)-1,N(l_2)-1,\cdots,N(l_p)-1;\cdots\right)}{N\left(L,N(l_1),N(l_2),\cdots,N(l_p);\cdots\right)} = \frac{\nu^{(1)}(l_1)\nu^{(1)}(l_2)\cdots\nu^{(1)}(l_p)}{(\nu^{(0)})^{p-1}}, \tag{17}$$

and

$$\frac{P\left(L-1,N(l_1)-1\right)}{P\left(L,N(l_1)\right)} = \frac{1}{n(l_1)}, \tag{18}$$

where dots after the semicolon in the denominator and numerator of the left-hand side of eq. (17) represent common parts. We need these ratios since the orbital $l_1$ at the site $i$, where orbitals $l_2,\cdots,l_p$ are occupied, should also be occupied before the hopping process. Therefore the other $N(l_i)-1$ $(i=1,\cdots,p)$ carriers must be on the other $L-1$ sites.

Finally, we obtain the result for $r_{c_{l_1}}$,

$$r_{c_{l_1}} = \frac{\nu^{(1)}(l_1)}{n(l_1)}\Big[1 + \\ + \sum_{\substack{p\geq 2\\ \{l_2,\cdots,l_p\}(\neq l_1)}} \eta^{(p)}\left(\{l_1,\cdots,l_p\}\right)\eta^{(p-1)}\left(\{l_2,\cdots,l_p\}\right)\frac{\nu^{(1)}(l_2)\cdots\nu^{(1)}(l_p)}{(\nu^{(0)})^{p-1}}\Big]. \tag{19}$$

In the same fashion, in terms of

$$\frac{N\left(L-1,N(l_{1'}),N(l_{2'})-1,\cdots,N(l_{p'})-1;\cdots\right)}{N\left(L,N(l_{1'}),\cdots,N(l_{p'});\cdots\right)} = \frac{\nu^{(0)}\nu^{(1)}(l_{2'})\cdots\nu^{(1)}(l_{p'})}{(\nu^{(0)})^{p'-1}}, \tag{20}$$

and

$$\frac{P\left(L-1,N(l_{1'})\right)}{P\left(L,N(l_{1'})\right)} = \frac{1}{1-n(l_{1'})}, \tag{21}$$

one obtains

$$r_{c^\dagger_{l_{1'}}} = \frac{\nu^{(0)}}{1-n(l_{1'})}\Big[1 + \\ + \sum_{\substack{p'\geq 2 \\ \{l_{2'},\cdots,l_{p'}\}(\neq l_{1'})}} \eta^{(p')}\left(\{l_{1'},\cdots,l_{p'}\}\right)\eta^{(p'-1)}\left(\{l_{2'},\cdots,l_{p'}\}\right)\frac{\nu^{(1)}(l_{2'})\cdots\nu^{(1)}(l_{p'})}{(\nu^{(0)})^{p'-1}}\Big]. \quad (22)$$

Substituting eq. (13) to eqs. (19) and (22) for $l_1 = l_{1'} = l$, we finally conclude the result (8) for $q(l) = r_{c^\dagger_l} r_{c_l}$.

Generally in the case $l \neq l'$, asymmetry arises between $r_{c^\dagger_{l'}}$ and $r_{c_l}$, or, one obtains different factors $q_{l'l}$ and $q_{ll'}$ for $\langle c^\dagger_{jl'} c_{il}\rangle$ and $\langle c^\dagger_{il} c_{jl'}\rangle$, respectively. These should be the same because of the Hermite character of the Hamiltonian. Thus in this situation, one may instead use their average $q = (q_{l'l} + q_{ll'})/2$ for both of $\langle c^\dagger_{jl'} c_{il}\rangle$ and $\langle c^\dagger_{il} c_{jl'}\rangle$. In the same manner, the $q$ factors for $\langle c^\dagger_{jl'} c^\dagger_{il}\rangle$ and $\langle c_{il} c_{jl'}\rangle$ take different forms. In this case, however, one can use their geometrical mean since these factors always appear pairwise as a product in physical terms.

Notwithstanding general treatment, compared with the method of Vollhardt,[3] our derivation presented above is not only simple but transparent with respect to the physical meaning of respective terms contributing to the $q$ factor. This is due to observation made at (16); we treated the two sites involved separately, while usually these are treated altogether. In particular, the square root $\sqrt{\nu^{(p)}}$ appears in eq. (8) in place of $\eta^{(p)}$, eq. (13), while squared $\eta^{(p)}$ there stems from the norm $\langle\Psi|\Psi\rangle$, eq. (10). Therefore our derivation validates our previous interpretation of $q(l)$ as a sum of products of probability amplitudes $\sqrt{\nu^{(p)}}$.

In passing, we end this article with a comment on the metal-insulator transition of the type noted first by Brinkman and Rice.[4] Summing eq. (6) over $l_1$, we obtain

$$\begin{aligned} n &= \sum_{l_1} n(l_1) = \sum_{l_1}\nu^{(1)}(l_1) + \sum_{l_1}\sum_{p(\geq 2)}\sum_{\{l_2,\cdots,l_p\}(\neq l_1)}\nu^{(p)}(l_1,l_2,\cdots,l_p) \\ &= \sum_{l_1}\nu^{(1)}(l_1) + \sum_{p(\geq 2)}\sum_{\{l_1,\cdots,l_p\}} p\,\nu^{(p)}(l_1,l_2,\cdots,l_p) \\ &= \sum_{p}\sum_{\{l_1,\cdots,l_p\}} p\,\nu^{(p)}(l_1,l_2,\cdots,l_p). \end{aligned} \quad (23)$$

If the on-site interaction is strong enough, one may consider only configurations which have $p-1$, $p$ and $p+1$ carriers on a single site, where an integer $p$ is selected so that $p-1 < n < p+1$. Then, if we set probabilities of the other configurations as zero, eqs. (23), (7) and (8) become

$$\begin{aligned} n = &\sum_{\{l_1,\cdots,l_{p-1}\}}(p-1)\,\nu^{(p-1)}(l_1,l_2,\cdots,l_{p-1}) + \sum_{\{l_1,\cdots,l_p\}} p\,\nu^{(p)}(l_1,l_2,\cdots,l_p) \\ &+ \sum_{\{l_1,\cdots,l_{p+1}\}}(p+1)\,\nu^{(p+1)}(l_1,l_2,\cdots,l_{p+1}), \quad (24) \\ 1 = &\sum_{\{l_1,\cdots,l_{p-1}\}}\nu^{(p-1)}(l_1,l_2,\cdots,l_{p-1}) + \sum_{\{l_1,\cdots,l_p\}}\nu^{(p)}(l_1,l_2,\cdots,l_p) \end{aligned}$$

$$+ \sum_{\{l_1,\cdots,l_{p+1}\}} \nu^{(p+1)}(l_1, l_2, \cdots, l_{p+1}), \tag{25}$$

and

$$q(l_1) = \frac{1}{n(l_1)\,(1-n(l_1))}\Bigg( \sum_{\{l_2,\cdots,l_p\}(\neq l_1)} \sqrt{\nu^{(p)}(l_1,\cdots,l_p)}\sqrt{\nu^{(p-1)}(l_2,\cdots,l_p)} + \sum_{\{l_2,\cdots,l_{p+1}\}(\neq l_1)} \sqrt{\nu^{(p+1)}(l_1,\cdots,l_{p+1})}\sqrt{\nu^{(p)}(l_2,\cdots,l_{p+1})}\Bigg)^2. \tag{26}$$

Subtracting $p$ times eq. (25) from eq. (24), we get

$$n - p = -\sum_{\{l_1,\cdots,l_{p-1}\}} \nu^{(p-1)}(l_1, l_2, \cdots, l_{p-1}) + \sum_{\{l_1,\cdots,l_{p+1}\}} \nu^{(p+1)}(l_1, l_2, \cdots, l_{p+1}). \tag{27}$$

For the Brinkman-Rice transition that $q(l)$, eq. (26), to vanish, the two terms in the right-hand side of eq. (27) must vanish at a time. This is because $\nu^{(p)}$ in eq. (26) generally remain non-zero to accommodate $n$ particles per site, or to meet eq. (24). (Note that $\nu^{(p)} \geq 0$ for any $p$.) Thus we conclude that the Brinkman-Rice transition occurs only when the carrier density $n$ equals an integer $p$.[5)]

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[1] T. Okabe: J. Phys. Soc. Jpn. **65** (1996) 1056.

[2] Recently, Bünemann and Weber came to the same conclusion; J. Bünemann and W. Weber: preprint (SISSA: cond-mat/9611031).

[3] D. Vollhardt: Rev. Mod. Phys. **56** (1984) 99.

[4] W. F. Brinkman and T. M. Rice: Phys. Rev. **B2** (1970) 4302.

[5] J. P. Lu: Phys. Rev. **B49** (1994) 5687; preprint (SISSA: cond-mat/9601133).